Gradient Library Calibration and the NCMC Informatics Effort

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Agenda

Calibration of Gradient Combi Libraries

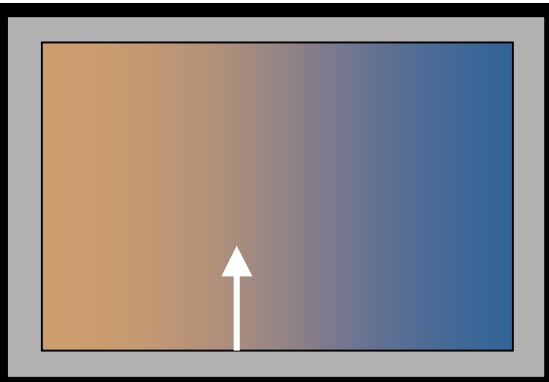
- Use and Utility of Spatial Reference Grids
- Implications on Informatics
- *Practical Knowledge for Gradient Techniques*

NCMC Informatics Project

- Purpose and Strategy
- *Transparent, Useable Examples* $\rightarrow$ *Informatics Standards*

Why is Library Calibration Necessary?

The Cartoon Gradient



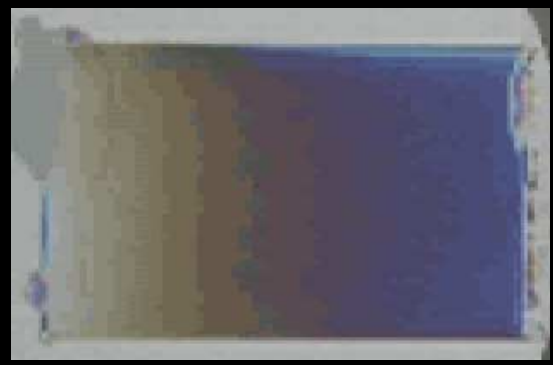
Linear gradient
- one slope
- even along “y”

Known dimension and orientation

Known scope

Defect Free

Reality



Non-linear gradient
- Variable slopes in x and y

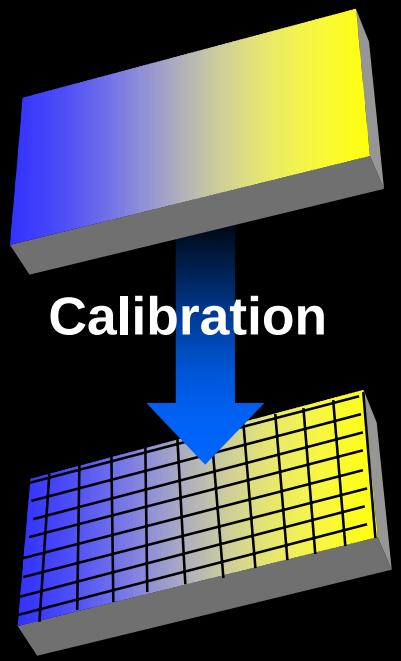
Arbitrary orientation

Scope approximate

Defects Present

Library Calibration:

What is needed before a gradient library is useful for combinatorial research?

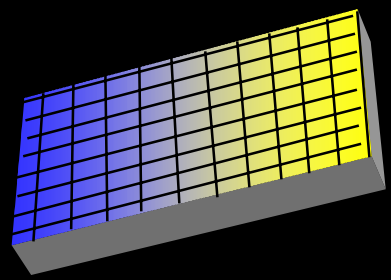


- Spatial reference grid
  - Mesh of calibration measurements
- Flaw/defect criteria met
- Library scope overlaps known phenomenon
  - "Built-in" standard
- Scope and tolerance of library known
  - Evaluation of uncertainty

Process combi gradient libraries so they can be "handled" like discrete combi libraries

Spatial Reference Grids (SRG):

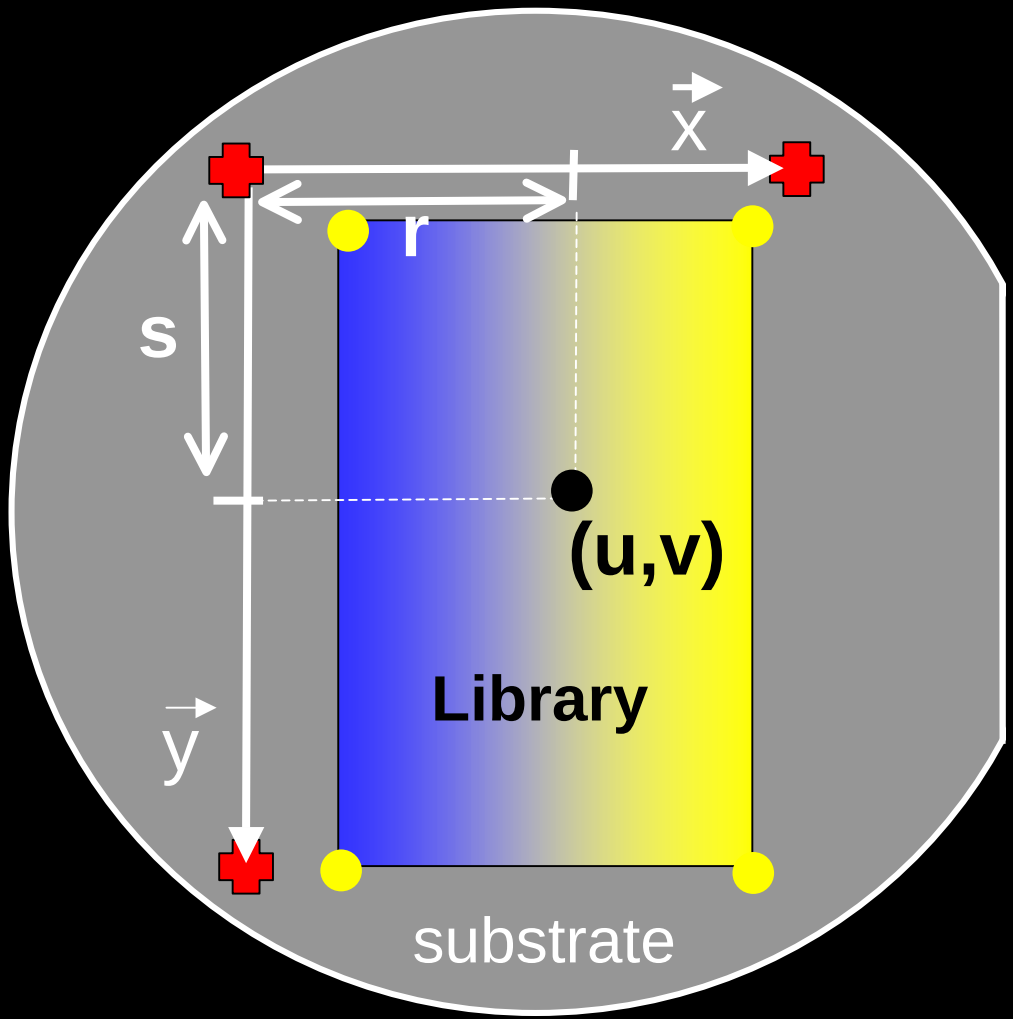
Define the sample space with respect to a reference or “fiduciary” marking system



Spatial Reference Grids Enable:

- Organization/Automation of sample measurements
- Definition of non-linear gradients (almost all!).
- Alignment/Registry of multiple gradients
- Definition and measurement of gradient steepness
- Interpolation: “zooming in”, “isobars”
- Library transfer (e.g. to another substrate)

Elements of a Spatial Reference Grid



3-Point Fiduciary Mark System

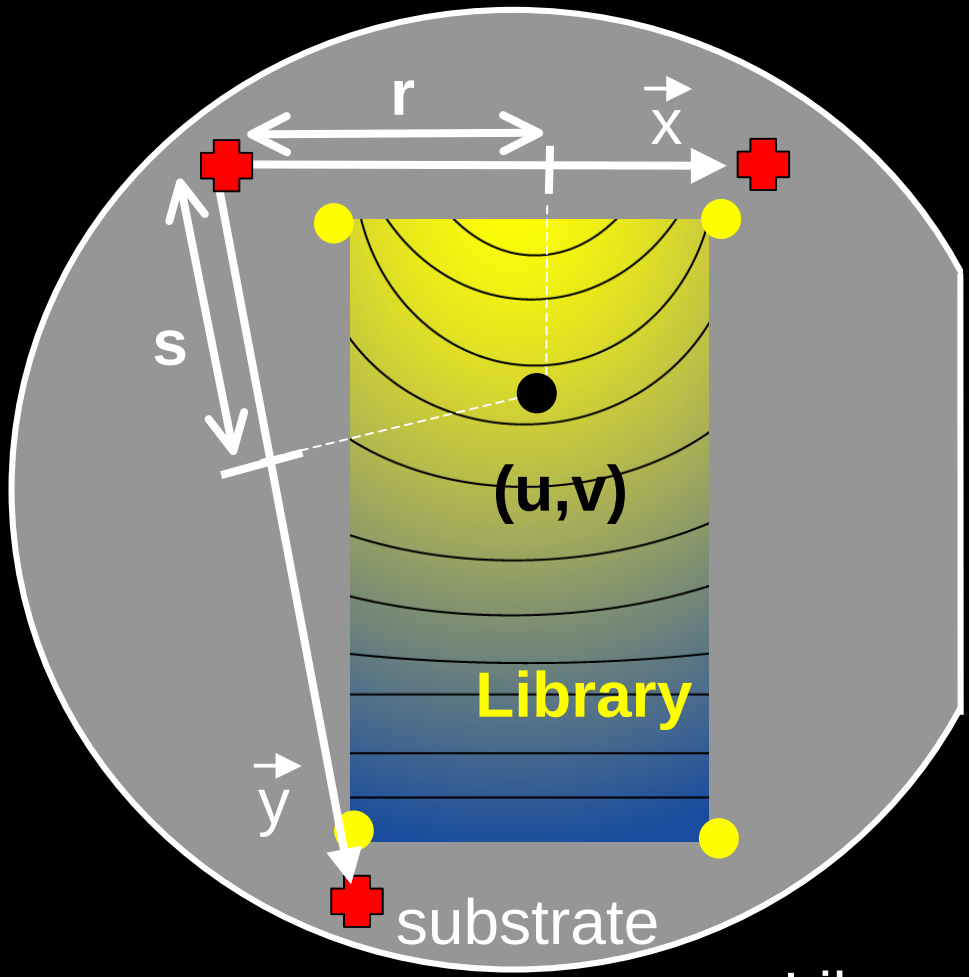
Reference Vectors $\vec{x}$ & $\vec{y}$

Coordinate System

$$(u,v) = \left(r \frac{\vec{x}}{|\vec{x}|}, s \frac{\vec{y}}{|\vec{y}|} \right)$$

Library boundaries defined in terms of **(u,v)**

Elements of a Spatial Reference Grid



- Reference vector analysis accommodates non-orthogonal fiduciary systems
- The SRG defines points for a mesh of calibration measurements.

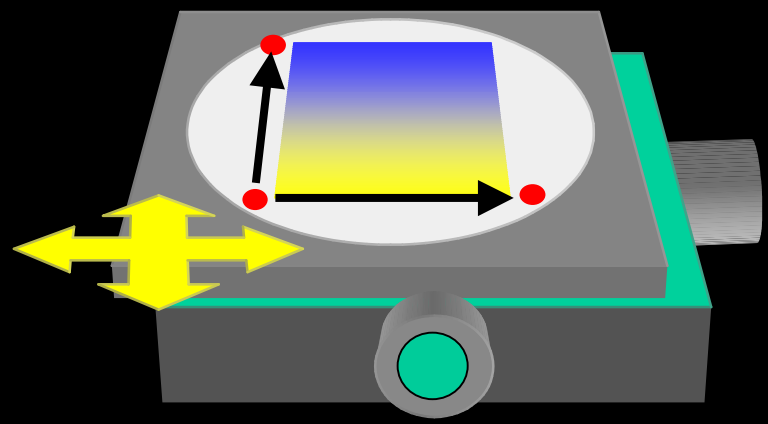
This mesh defines the library variable space.

Library boundaries ●

Fiduciary Marks ✚

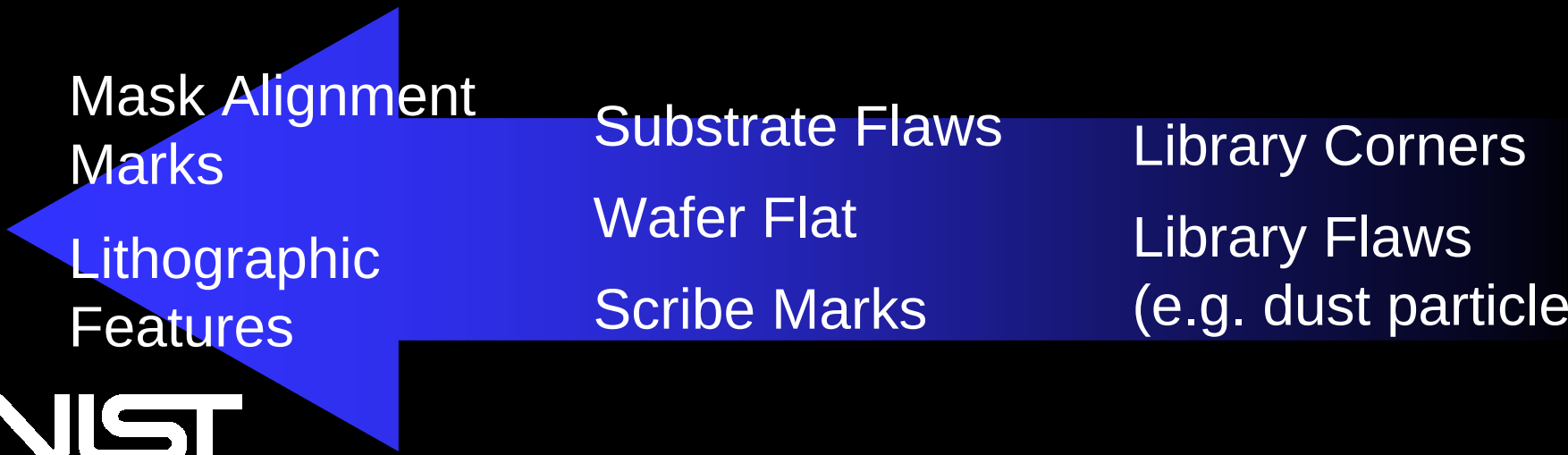
SRG Pointers:

- Use xy-stages to define reference vectors
  - let calibrated stages work for you
- Program automation tools to work within reference system
  - Alignment with reference system should always be the first step of automated analysis



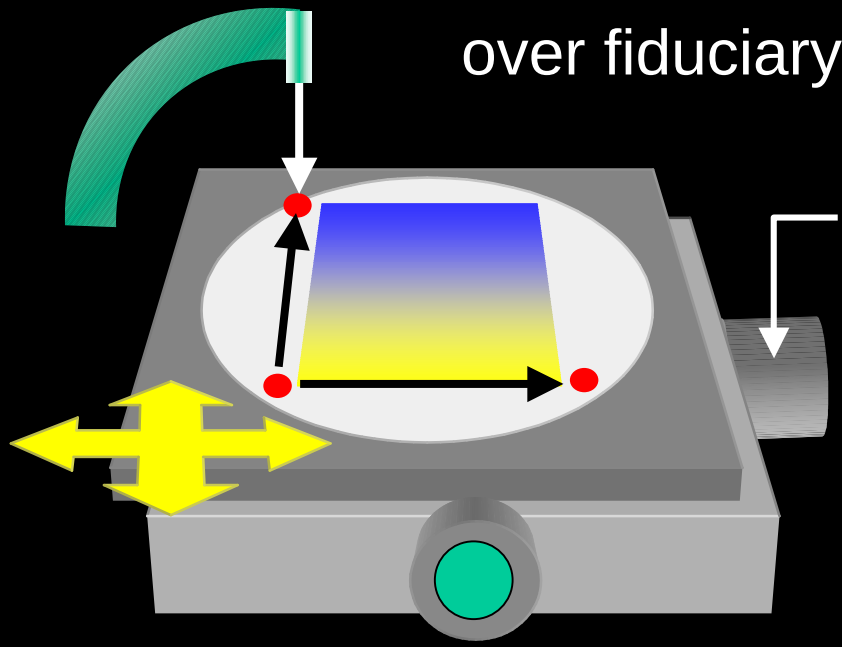
Notes on Fiduciary Marks:

- Fiduciary marks may be within library borders
  - allows for easy library transfer
- Factors to consider when choosing fiduciary marks:
  - Permanence
  - Readily identified/recognized?
  - Size
  - Calibration measurement technique (ellipsometry? OM?)



xy-stages and the SRG :

Translation stages with *encoded stepper motors* provide a convenient means of SRG definition

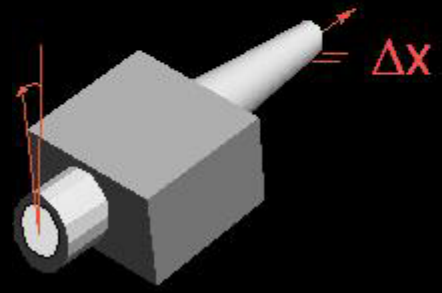


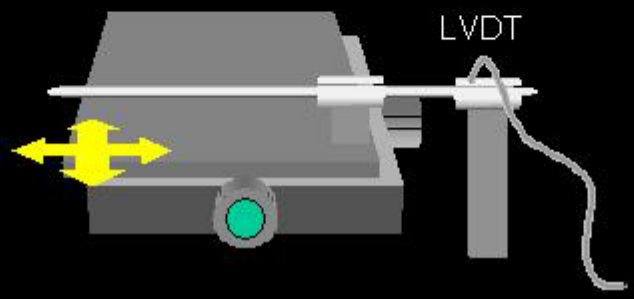
1. Center measurement tool (here interferometer) over fiduciary mark using stage motors
2. Record motor positions
3. Repeat for each mark
4. Define reference vectors
5. Take calibration measurements on grid defined by reference vectors

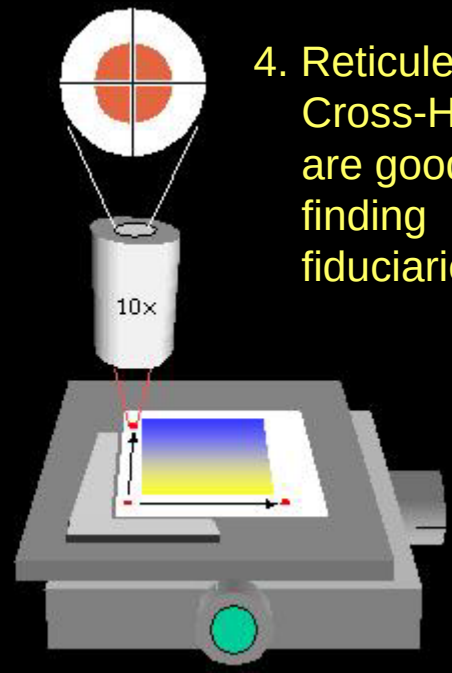
SRG and Sources of Error

1. Motor step size
2. Stage following error
3. Sample Alignment
4. Fiduciary Mark Registration

} From manufacturer







4. Reticule / Cross-Hairs are good for finding fiduciaries

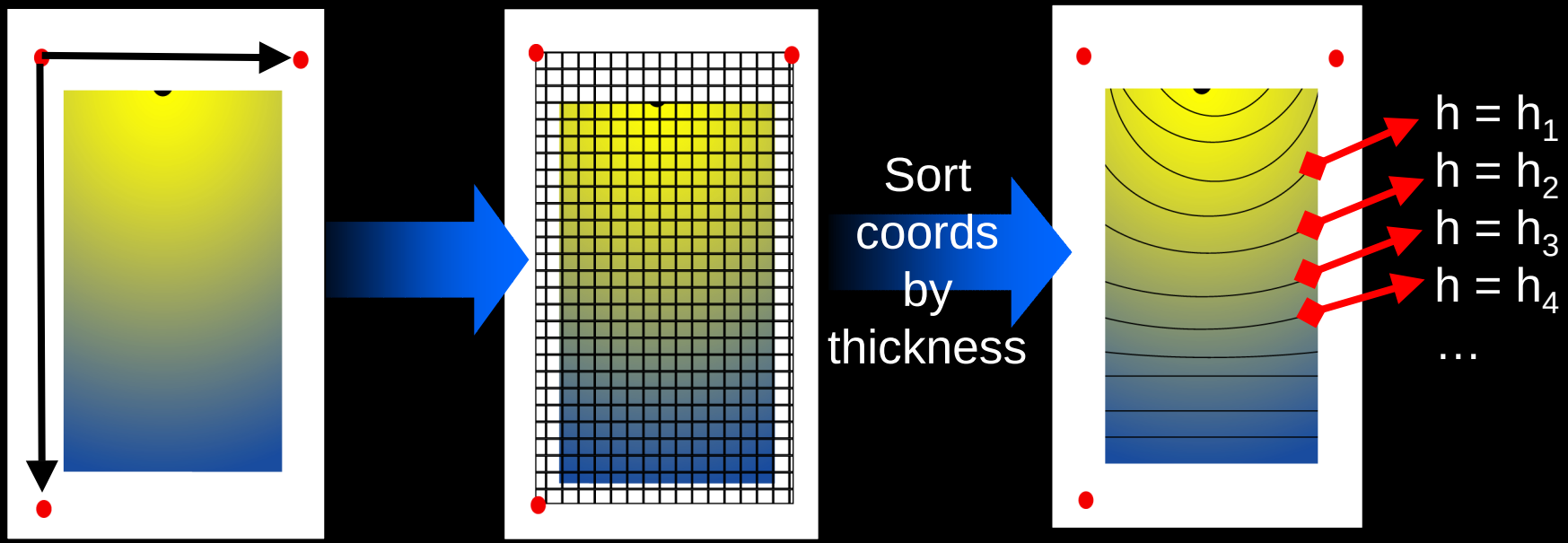
1. Motor step size:
   Should be < 5% of measurement footprint

2. Stage following Error:
   - Tune motors properly
   - External fixed encoders to accurately determine position

3. Sample Alignment:
   Jig/Slot for reproducible sample placement

Iso-parametric Contour Lines:

Non-linear spatial distribution → Linear parameter space



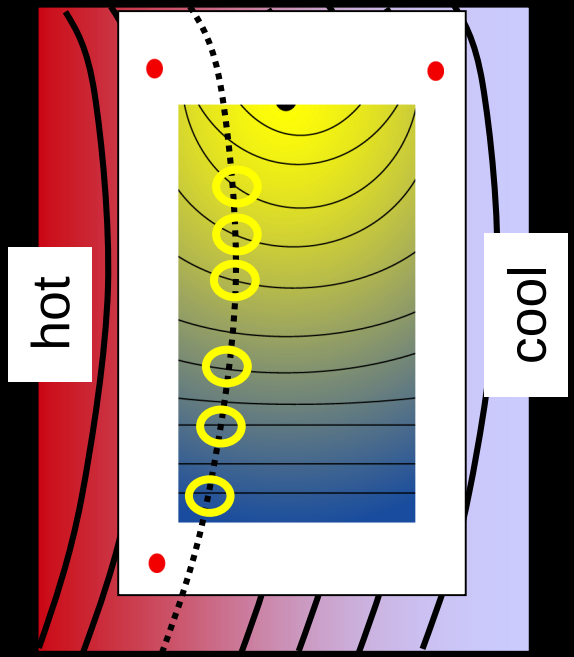
Non-linear thickness gradient

Thickness measurements on SRG

Contours delineate coordinates with equal thickness

Iso-parametric Contour Lines:

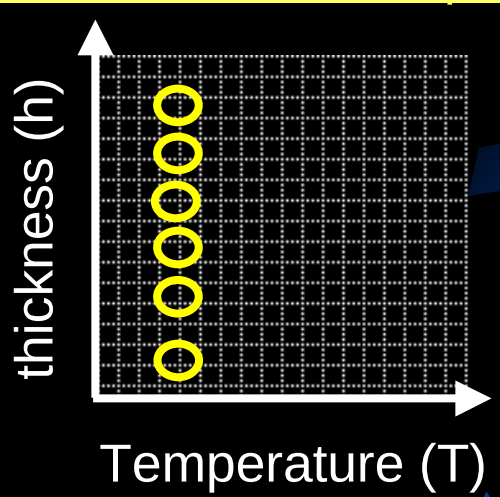
Deconvolution of crossed non-linear gradients

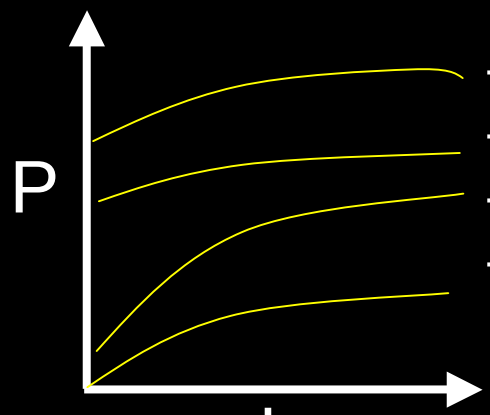


Calibrated gradient hot stage

Contour line intersections

Linear Parameter Space





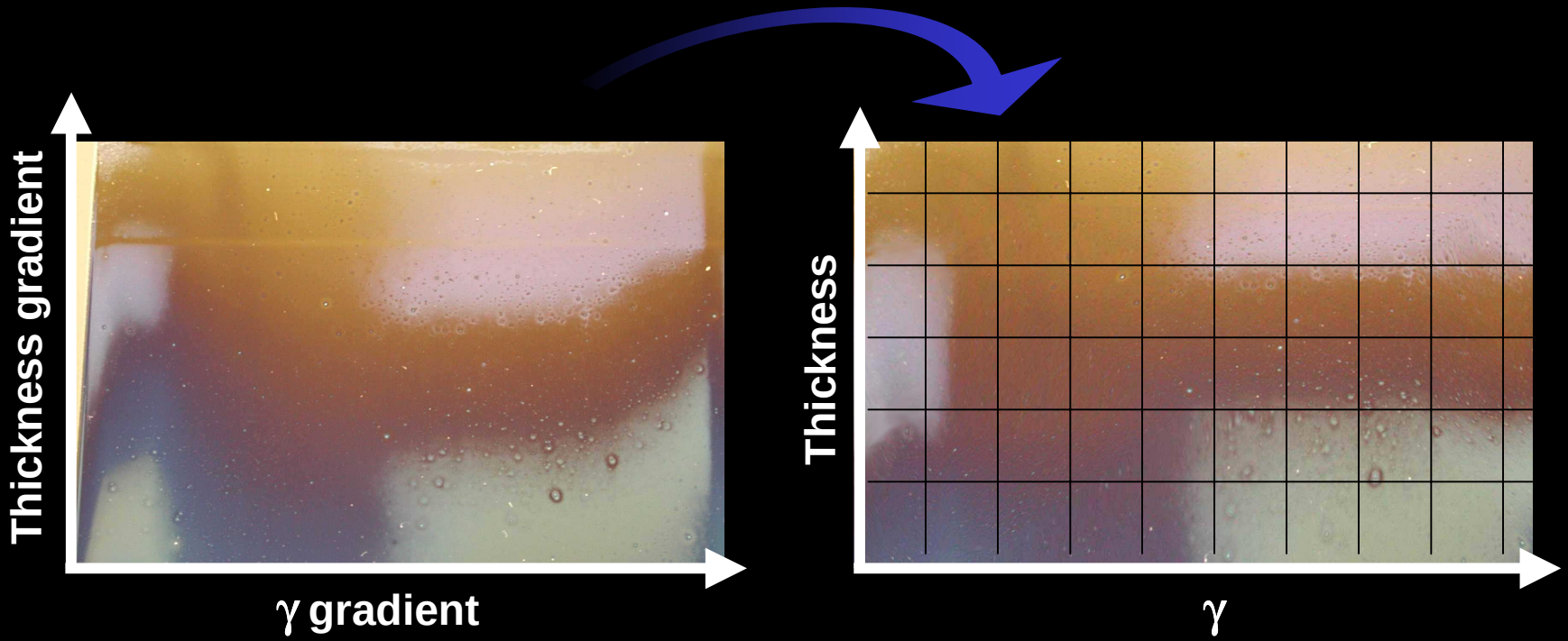
$T = T_1$
$T = T_2$
$T = T_3$
$T = T_4$

Rational data organization and presentation

Block Copolymer Film Library

A.P. Smith, A. Sehgal, J.F. Douglas, A. Karim, E.J. Amis

***Macromol. Rapid Commun.* 24(1), *131,* 2003**

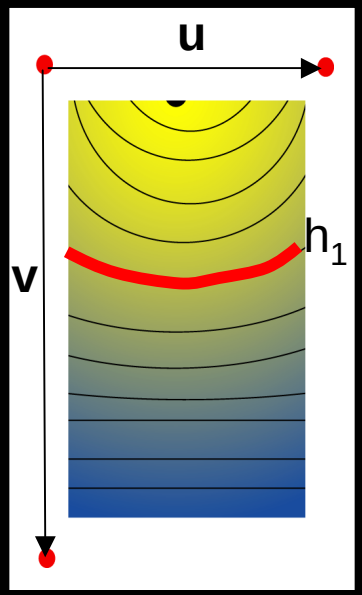


As fabricated: non-linearities in thickness and surface energy gradients

Calibrated: contour lines used to process library into orthogonal coordinates

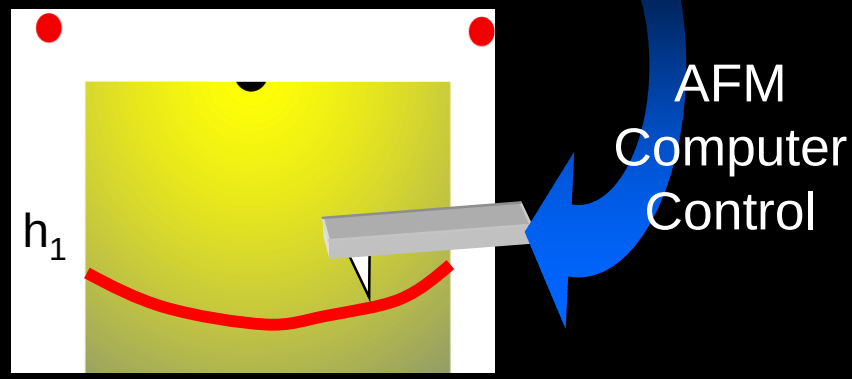
Utility of Contour Lines:

Problem: Thickness "h_1" is of particular interest. How can we concentrate further analysis on this thickness?



Solution:

1) Generate iso-h contours using SRG and calibration mesh
2) Use h_1 contour line to generate coordinates (u,v) for which the thickness = h_1
3) Use h_1 coordinates as input for automation and informatics



Gradient Combi and Informatics Design

Key: Integration and Transfer of SRG System

- Automated Fabrication Tools work around SRG
  - Fiduciary marks defined during fabrication
  - SRG Defined during library calibration
- Database structured to carry SRG Vector System
  - Locations of fiduciary marks, especially origin
  - SRG unit vectors, rather than entire grid
- Analysis tools automatically query Database for SRG
  - Essential information for iso-parametric, orthogonal data set processing

NCMC Informatics Project

Transparent, Usable Examples → Standards Development

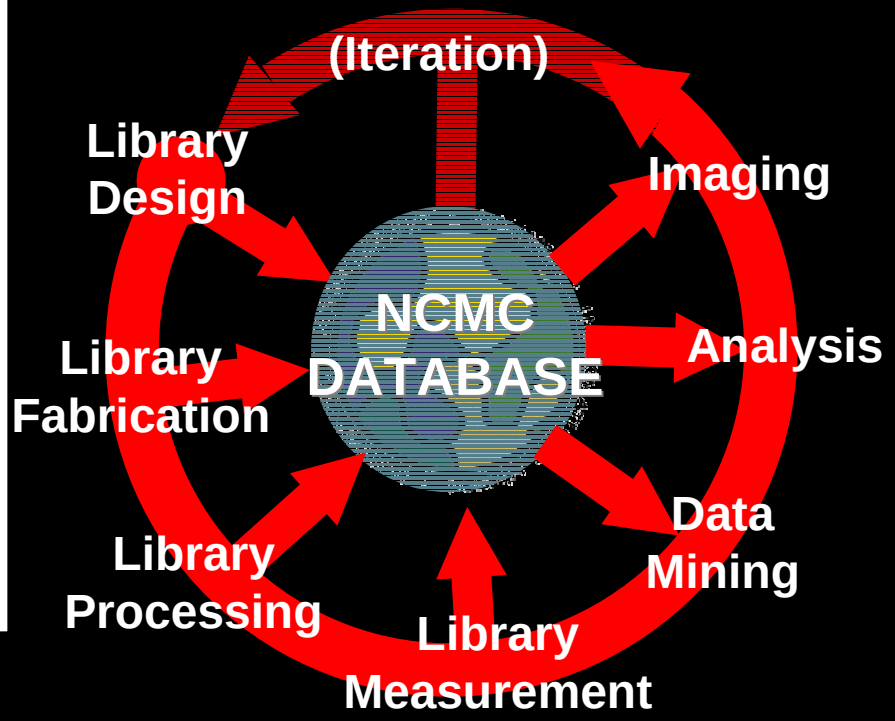
- Consolidation/Integration of NCMC automation and analysis software
  - Gradient Compatible
- Development of combi research database system:

Designed for transparency

Built on open source code

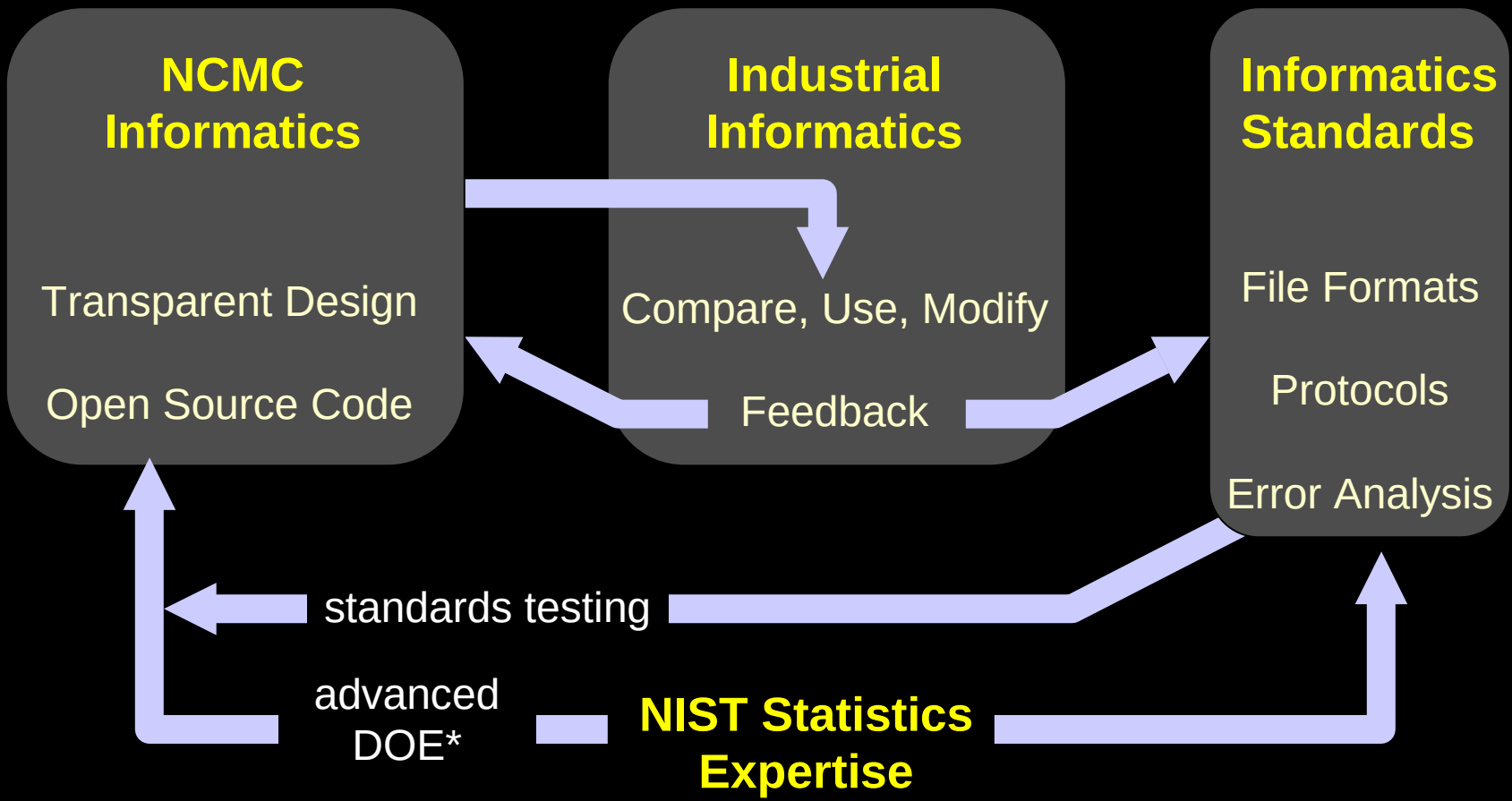
Web Access

Eventual public data mining



NCMC Informatics Project

Transparent, Usable Examples → Standards Development

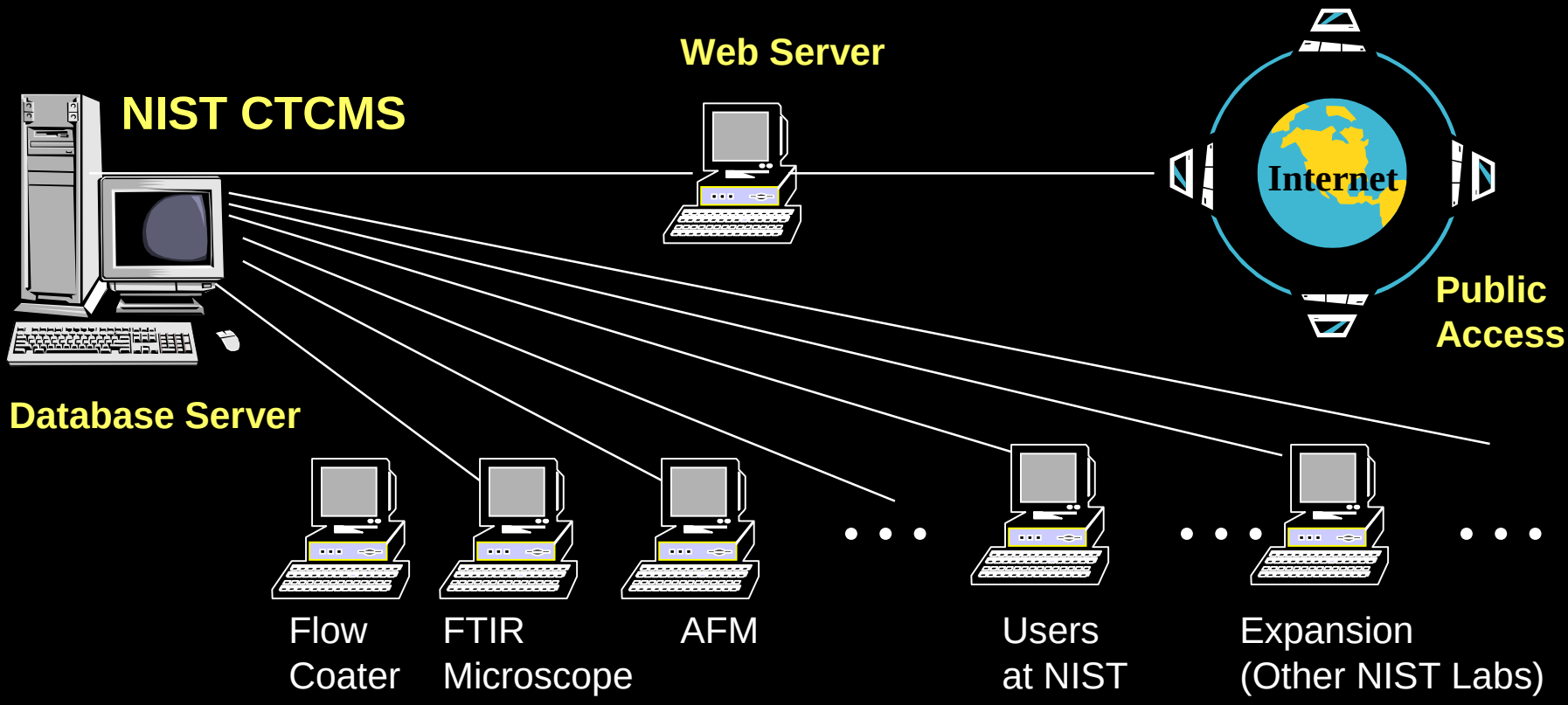


*Design of Experiments

Initial Phase: Infrastructure Deployment

NCMC Informatics Infrastructure development:

Dr. Wenhua Zhang (CUNY Staten Island, Dept. of Chem.)



NCMC Instruments and Analysis Software

This phase is nearing completion

NCMC Combi Informatics Workshop

w/ CTCMS and the Statistical Engineering Division

May 22,23 2003, NIST Gaithersburg, MD

Informatics Seminar

- Resource Integration
- DOE strategies
- Combi Error Analysis

→ Issues Defined

Informatics Standards Forum

- Research Industry
- Instrument Producers
- Software Providers

→ Issues Discussed

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http://www.nist.gov/combi

Contributors

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Thanks!